

Boat conformation in 2,5-substituted 1,3-dioxanes

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Abstract

The calculation of the energy equilibrium according to Pitzer between the chair and boat conformations in 2,5-substituted 1,3-dioxanes is presented, as well as the energies of the electrostatic dipole interactions. It is shown that the unsymmetrical boat conformation is stabilized in 2,5-dialkyl- and in 2,2-dimethyl-5-alkyl-5- α -alkoxyalkyl-1,3-dioxanes because of the presence of hetero atoms in the ring, because of the introduction of substituents in the 2 and 5 positions, and because of the interaction between the hybridized, unshared electron pairs of the oxygen atom at the apex of the boat with the hydrogen atom of the CH₂ group. © 1970 The Faraday Press, Inc.

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